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Evolution of the excess conductivity in slightly doped $YBa_2Cu_3O_{7-\delta}$ under high pressure

A. L. Solovjov^{1,2}, L. V. Omelchenko^{1,2}, R. V.Vovk³

¹B. I.Verkin Institute for Low Temperature Physics and Engineering of National Academy of Science of Ukraine, 47 Lenin ave., 61103 Kharkov, Ukraine

²International Laboratory of High Magnetic Fields and Low Temperatures, 95 Gajowicka Str., 53-421, Wroclaw, Poland ³Physics Department, V. N. Karazin Kharkiv National University, Svobody Sq. 4, 61022 Kharkiv, Ukraine

The influence of hydrostatic pressure up to P=1.05 GPa on resistivity, excess conductivity $\sigma'(T)$ and pseudogap (PG) $\Delta^*(T)$ in slightly doped single crystals of YBa₂Cu₃O_{7.8} (T_c(P = 0) ≈49.2 K and $\delta \approx 0.5$) is studied. For the first time it is found that the BCS ratio $2\Delta^*/k_B T_c$ and PG Δ^* both increase with increasing external hydrostatic pressure at a rate $dln\Delta^*/dP \approx 0.37$ GPa⁻¹, implying an increase of the coupling strength with pressure. Simultaneously, the critical temperature T_c also increases with increasing pressure at a rate $dln\rho/dP = (-19\pm0.2)\%$ GPa⁻¹. Independently on pressure near T_c $\sigma'(T)$ is well described by the Aslamasov-Larkin and Hikami-Larkin fluctuation theories demonstrating 3D-2D crossover with increase of temperature. The crossover temperature T₀ determines the coherence length along the c-axis $\xi_c(0) = (3.43 \pm 0.01)$ Å at P=0 GPa, which decreases with pressure.

Keywords: Fluctuation conductivity, pseudogap, pressure, excess conductivity, YBaCuO single crystals.

В работе исследовано влияние гидростатического давления до P=1.05 ГПа на удельное сопротивление, избыточную проводимость $\sigma'(T)$ и псевдощель (ПЩ) $\Delta^*(T)$ в слабо допированном монокристалле $YBa_2Cu_3O_{7.6}$ с ($T_c(P=0) \approx 49.2$ К и $\delta \approx 0.5$). Впервые обнаружено, что соотношение БКШ $2\Delta^*/k_BT_c$ и ПЩ Δ^* возрастают с ростом давления как dln $\Delta^*/dP \approx 0.37$ GPa⁻¹, указывая на увеличение силы связи. Показано, что критическая температура T_c также увеличивается с увеличение P как dT_c/dP=+5.1 K·ГПа⁻¹, в то время как удельное сопротивление $\rho(300K)$ уменьшается как dln $\rho/dP = (-19\pm0.2)\%$ ГПа⁻¹. Независимо от давления вблизи T_c $\sigma'(T)$ хорошо описывается флуктуационными теориями Асламазова–Ларкина и Хиками– Ларкина, демонстрируя 3D- 2D кроссовер при увеличении температуры. Температура кроссовера T_0 позволяет определить длину когерентности ξ_c (0) = (3.43\pm0.01)Å при P=0 ГПа, которая уменьшается с давлением.

Ключевые слова: Флуктуационная проводимость ,псевдощель, давление, избыточная проводимость, монокристаллы YBaCuO.

В роботі досліджено вплив гідростатичного тиску до P = 1.05 ГПа на питомий опір, надлишкову провідність $\sigma'(T)$ і псевдощілину (ПЩ) $\Delta^*(T)$ в слабодопованому монокристалі $YBa_2Cu_3O_{7,\delta}$ з (T_c (P = 0) \approx 49.2 K і $\delta\approx$ 0.5). Вперше виявлено, що співвідношення БКШ $2\Delta^*/k_BT_c$ і ПЩ $\Delta^*(T)$ зростають зі збільшенням тиску, як dln $\Delta^*/dP \approx 0.36$ GPa⁻¹, маючи на увазі збільшенням сили зв'язку з тиском. Показано, що критична температура збільшується зі збільшенням тиску dT_c/dP=+5.1 K·ГПа⁻¹, в той час, як $\rho(300)$ К зменшується dln $\rho/dP = (-19\pm0.2)$ ГПа⁻¹. Незалежно від тиску поблизу T_c $\sigma'(T)$ добре описується флуктуаційними теоріями Асламазова-Ларкіна і Хікамі- Ларкіна, демонструючи 3D- 2D кросовер при збільшенні температура з тиском. Ключові слова: Флуктуаційна провідність, псевдощілина, тиск, надлишкова провідність, монокристали YBaCuO.

Introduction

Pseudogap (PG), which is opening in the excitation spectrum at the characteristic temperature $T^*>> T_c$, where T_c is the resistive transition temperature, still remains one of the most interesting and intriguing property of high- T_c cuprate superconductors (HTS's or cuprates) [1–3]. It is believed that the proper understanding of the PG physics has to promote deciphering the basic pairing mechanism in the HTS's [1,2]. Since the observation of a large pressure dependence of T_c in the La–Ba–Cu-0 system [4], pressure plays an important role in the study of HTS's. In contrast to conventional superconductors, dT_c/dP for the high- T_c superconductors appears to be in most cases positive whereas $dlnp_{ab}/dP$ is negative and relatively large [5-8]. Applied pressure produces a reduction in lattice volume which promotes ordering [5] and this appears to lead to positive dT_c/dP observed in experiment. The interpretation of the pressure effect on ρ is rather uncertain, since the nature of the transport properties for HTS's is not clear yet. The dominant contribution to the conductivity is known to come from the CuO₂ planes which are interconnected by a relatively weak transfer interaction. Most likely pressure leads to the increase of the charge concentration n_f in the CuO₂ planes, which in turn has to affect both T_c and $\rho(T)$. The theoretical approach to the hydrostatic-pressure effects on the resistance of HTS's is discussed in Ref. [5]. There are also several papers in which the influence of pressure on the fluctuation conductivity (FLC) was studied in HTS's compounds [6-8]. But as far as we know no detailed study of pressure influence on pseudogap in the high-Tc oxides has been carried out up to now.

In the paper we report on the in-plane resistivity ρ_{ab} (T) measurements under hydrostatic pressures up to P = 1.05 GPa in slightly doped YBa₂Cu₃O_{7- $\delta}$} (YBCO) single crystals with the oxygen index 7- δ ~ 6.5 and T_c = 49.2K at P = 0 GPa. We studied the excess conductivity $\sigma'(T)$ and focused on the temperature dependence of FLC. From the analysis of the excess conductivity the magnitude and temperature dependence of pseudogap $\Delta^*(T)$ with and without pressure were finally derived. The analysis was performed within our Local Pair (LP) model [1,9,10] as discussed in details in the text.

Experiment

The YBa₂Cu₃O_{7.8} (YBCO) single crystals were grown with the self-flux method in a gold crucible, as described elsewhere [11-14]. For electrical resistance measurements were selected crystals of rectangular shape with typical dimensions of 3×5×0.3mm³. The smallest parameter of the crystal corresponds to the c-axis. To obtain samples with given oxygen content, the crystals were annealed in an oxygen atmosphere as described in Refs. [14,15]. The electrical resistance in the ab-plane, $\rho_{ab}(T) \equiv \rho(T)$, was measured in the standard four-probe geometry with a dc current up to 10mA in the regime of fully automated data acquisition. The measurements were conducted in the temperature sweep mode, with a rate of 0.1 K/min near T and about 5 K/min at T >> T_c . The hydrostatic pressure was generated inside an autonomous chamber (piston-cylinder type) as described elsewhere [13,14]. A manganin gauge made of a 25 Ω wire was used to determine the applied pressures. The temperature measurements were performed using a copper-constantan thermocouple mounted at sample level on the outside of the chamber [13].

Figure 1 displays the temperature dependencies of the resistivity $\rho(T)$ of the studied YBCO single crystal measured at P = 0 GPa (curve 1) and P = 1.05 GPa (curve 2), respectively. The curves have an expected S-shaped form being typical for the slightly doped YBCO films [1,16] and single crystals [17,18]. Above T*~ 260 K $\rho(T)$ varies linearly with T at a rate $d\rho/dT = 2.48 \ \mu\Omega cmK^{-1}$ and $d\rho/dT = 2.08 \ \mu\Omega cmK^{-1}$ for the pressures P = 0 and 1.05 GPa, respectively. (Note that 1 GPa = 10 kbar). This linearity is characteristic for the normal state of cuprates



Fig. 1. Temperature dependence of ρ of YBa₂Cu₃O_{7.8} (7 – δ ~6.5) single crystal at P=0 GPa (curve 1 dots) and 1.05 GPa (curve 2, semicircles). Inserts display the way of T* determination at P=0 GPa using (ρ (T) – ρ_0))=aT criterion.

[16-20]. The slopes were determined by the computer linear fitting which results in the rather good linearity in the stated temperature range with the standard error of about (0.009±0.002) at all applied pressures. The PG temperature T* is taken at the point where the experimental resistivity curve starts to downturn from the linear behavior at the higher temperatures designated by the dashed lines in the figure. The more precise approach for the T* determination is to use $[\rho(T) - \rho_0]$ =aT criterion [21]. Now T* is the temperature at which $[\rho(T) - \rho_0]/aT$ downturns from 1 as shown in insert in Fig. 1. Both approaches give the same T*'s.

The relative diminution of $\rho(T)$ as a function of pressure is practically temperature independent above 260 K and amounts to $dlnp(300K)/dP = (-19\pm0.2)\%$ GPa⁻¹. This value is in agreement with results obtained for different cuprates [5-8,13]. Simultaneously, the critical temperature T also increases with increasing pressure at a rate dT/ dP=+5.1 K·GPa⁻¹ which is in a good agreement with our results for slightly doped (SD) HoBCO single crystals where $dT_/dP=+4$ K·GPa⁻¹ is found [22]. The same $dT_/$ dP=+4 K·GPa⁻¹ was observed by pressure experiments in SD polycrystalline YBa₂Cu₃O_{7- δ} (7 - δ ~ 6.6) using a muon spin rotation (µSR) technique [23]. The result confirms the expressed assumption that in cuprates both ρ diminution and T_c increase occur likely at the expense of the increase of the charge carrier density n_f in the CuO₂ planes under pressure. Meanwhile, it is likely that the oxygen vacancies in the slightly doped cuprates provide the possibility for the more easy redistribution of n_eas compared with optimally doped samples where the number of vacancies is small and n_{f} is, in turn, rather large [1,2,24].

Results and discussion

Below the PG temperature T* the resistivity curves

at all applied pressures deviate down from the linear $\rho(T)$ observed at the higher temperatures (Fig.1). This leads to appearance of the excess conductivity

$$\sigma'(\mathbf{T}) = \sigma(\mathbf{T}) - \sigma_{\mathbf{N}}(\mathbf{T}) = \left[1/\rho(\mathbf{T})\right] - \left[1/\rho_{\mathbf{N}}(\mathbf{T})\right], (1)$$

where $\rho_N(T) = aT + \rho_0$ is the linear normal state resistivity extrapolated to low T region (dashed lines in the figure). Accordingly, $a=d\rho/dT$ and ρ_0 is the intercept with the y-axis. This procedure of the normal state resistivity determination is justified in Ref. [20] and is of a common occurrence now [21,25-27]. We will mainly perform analysis for the sample Y0 (P=0) and compare results with those obtained for the sample Y6 (with P=1.05 GPa applied for five days), as well as with results obtained for different cuprates [5-7]. Naturally, the same analysis has been performed at all applied pressures.

To begin with the analysis, the mean field critical temperature mf has to be found. Here $T_c^{mf} > T_c$ is the critical temperature in the mean-field approximation, which separates the FLC region from the region of critical fluctuations or fluctuations of the superconducting (SC) order parameter Δ directly near T_c (where $\Delta < kT$), neglected in the Ginzburg-Landau (GL) theory [28]. In all equations used in the analysis the reduced temperature

 $\varepsilon = \left(T - T_c^{mf} \right) / T_c^{mf}$ (2)



Fig. 2. $\ln \sigma'$ vs lnɛ at P=0GPa (panel a, dots) and P=1.05 GPa (panel b, circles) compared with the fluctuation theories: 3D AL (dashed line 1); MT with d = d1 (solid curve 2).

is exploited. Thus, the correct determination of T_c^{mf} [26] is decisive in the FLC and PG calculations. Within the LP model it was convincingly shown that near T_c FLC (Fig. 2, dots (P= 0 GPa) and circles (P= 1.05 GPa)) is always extrapolated by the standard equation of the Aslamasov-Larkin (AL) theory [29] (Fig. 2, dashed line 1), which determines FLC in any 3D system:

$$\sigma'_{AL3D} = C_{3D} \frac{e^2}{32h\xi_c(0)} \varepsilon^{-1/2} .$$
 (3)

Here ξ_c is a coherence length along the c-axis, d is a distance between conducting layers [30,31], and C_{3D} is a numerical factor used to fit the data by the theory [1,25,26]. This means that the conventional 3D FLC is realized in HTS's as T draws near T_c [1,30,31] providing the way for T_c^{mf} determination. From Eq. (3), one can easy obtain $\sigma'^{-2} \sim \epsilon \sim T - T_c^{mf}$. Evidently, $\sigma'^{-2}(T) = 0$ when $T = T_c^{mf}$ [1,26,30]. The interception of the extrapolated linear $\sigma'^{-2}(T)$ with T-axis determines both T_c^{mf} =50.2 K and, consequently, ϵ .

Figure 2 shows σ' as a function of ε plotted in double logarithmic scale. Above T_c^{mf} and up to $T_0 = 54.4$ K ($\ln \varepsilon_0 =$ -2.45, P=0 GPa) $\ln \sigma'(\ln \varepsilon)$ is well described by Eq. (3) which is the straight line with the slope $\lambda = -1/2$ (Fig. 2, dashed line 1). Above the crossover temperature T_0 data deviates up from the AL line suggesting the crossover to the 2D behavior which corresponds to the Maki–Thompson (MT) fluctuation contribution into FLC [31] (Fig. 2, solid curve 2). Thus, above T_0 and up to $T_{01} \approx 87.4$ K ($\ln \varepsilon_{01} \approx -0.3$) $\ln \sigma'$ ($\ln \varepsilon$) is well fitted by the MT term of the Hikami–Larkin (HL) theory [31]:

$$\sigma_{\rm MT}' = \frac{e^2}{8 dh} \frac{1}{1 - \alpha/\delta} \ln \left((\delta/\alpha) \frac{1 + \alpha + \sqrt{1 + 2\alpha}}{1 + \alpha + \sqrt{1 + 2\delta}} \right) \varepsilon^{-1} \quad (4)$$
In Eq. (4)

$$\alpha = 2 \left[\frac{\xi_{\rm c}(0)}{\rm d} \right]^2 \varepsilon^{-1} \tag{5}$$

is a coupling parameter,

$$\delta = \beta \frac{16}{\pi h} \left[\frac{\xi_{c}(0)}{d} \right]^{2} \kappa_{B} T \tau_{\phi}$$
(6)

is the pair-breaking parameter, and $\tau_{_{\phi}}$ that is defined by equation

$$\tau_{\phi}\beta T = \pi h/8k_{\rm B}\varepsilon = A/\varepsilon \tag{7}$$

is the phase relaxation time, and $A = 2.998 \cdot 10^{-12}$ sK. Factor $\beta = 1.203(1/\xi_{ab})$, where 1 is the mean-free path and ξ_{ab} (T) is the coherence length in the ab plane, considers the clean limit approach (1 > ξ) [1,31].

Evidently, at the crossover temperature $T_0 \sim \varepsilon_0$ the coherence length $\xi_{\tilde{n}}(T) = \xi_{\tilde{n}}(0)\varepsilon^{-1/2}$ is expected to

amount to d [9,30,31]. This yield $\xi_c(0)=d\sqrt{\varepsilon_0}$ and allows the possibility of $\xi_c(0)$ determination. Set d=11.67A, which is the c-axis lattice parameter in YBCO [33], one can easily obtain $\xi_c(0) = (3.43\pm0.02)$ Å and $\xi_c(0) = (2.91\pm0.02)$ Å for P=0 GPa and P=1.05 GPa, respectively. Both found $\xi_c(0)$ values are in a good agreement with those usually reported for SD YBCO [1,16,21]. ξ_c (0) is the important parameter of the PG analysis [1,2,8].

Accordingly, at $T=T_{01}$ (or $\varepsilon=\varepsilon_{01}$) $\xi_c(T)=d_1$, where d_1 is a distance between the conducting CuO₂ planes [9,19,30,31]. This yield $\xi_c(0)=d_1\sqrt{\varepsilon_{01}}$ and allows the possibility of d_1 determination since $\xi_c(0)$ has already been found. Finally, $d_1=(3.98\pm0.02)$ Å and $d_1=(3.37\pm0.02)$ Å were derived from the experiment for P=0 GPa and P=1.05 GPa, respectively. Revealed $d_1 = (3.98\pm0.02)$ Å is actually the inter-planar distance in YB₂Cu₃O_{6.65} at P=0GPa [33]. Both $\xi_c(0)$ and d_1 are found to decrease with pressure [5-7]. Within the LP model it is believed that below T_{01} $\xi_c(T)$ exceeds d_1 and couples the CuO₂ planes by Josephson interaction resulting in appearance of the 2D FLC of the MT type which lasts down to T_0 [1,9,30,31]. Correspondingly, below $T_0 \xi_c(T)$ exceeds d, and pairs can interact in the whole sample volume forming the 3D state now [30,31].

Finally, it turns out that just ε_{01} has to govern Eq. (4) now and its proper choice is decisive for the FLC analysis. Corresponding temperature T_{01} is introduced to determine the temperature range above T_c in which the SC order parameter wave function stiffness has to maintain [34, 35]. As it is clearly seen from the analysis, it is just the range of the SC fluctuations which obey the conventional fluctuation theories.

Pseudogap analysis

In HTS's pseudogap is manifested as a downturn of the longitudinal resistivity at T* from its linear behavior above T* [1, 2]. This results in appearance of the excess conductivity $\sigma'(T)$ (see Eq. (1)). It is well established now [1,2,10] that just the excess conductivity has to contain information about the PG. Evidently, to attain the information one needs an equation which specifies a whole experimental $\sigma'(T)$ curve, from T* down to T_c, and contains the PG in the explicit form. Besides, the dynamics of pair-creation and pair-breaking (see Eq. (9)) above T_c must be taken into account in order to correctly describe the experiment [1,9]. Due to the absence of a complete fundamental theory the equation for $\sigma'(T)$ has been proposed in Ref. [9] with respect to the local pairs:

$$\sigma'(\varepsilon) = \frac{e^2 A_4 \left(1 - \frac{T}{T^*}\right) \left(\exp(-\frac{\Delta^*}{T})\right)}{\left(16\hbar \xi_c(0) \sqrt{2\varepsilon_{c0}^* \sinh(2\varepsilon/\varepsilon_{c0}^*)}\right)} \tag{8}$$





Fig. 3. Temperature dependence of pseudogap parameter Δ^* of YBa₂Cu₃O_{6.5} single crystal at P=0 (curve 1, dots) and P=1.05 GPa (curve 2, semicircles). The data were analyzed with Eq. (11). Solid curve 3 indicates the result of such analysis performed at P=1.05 GPa but using the resistivity curve fitted by polynomial down to ~160K.

Here A_4 is a numerical factor which has the meaning of the C-factor in the FLC theory [1,10].

Solving Eq. (8) for the pseudogap $\Delta^{*}\left(T\right)$ one can readily obtain:

$$\Delta^{*}(T) = T \ln \frac{e^{2} A_{4} \left(1 - \frac{T}{T^{*}}\right)}{\sigma'(T) 16 \hbar \xi_{c}(0) \sqrt{2\varepsilon_{c0}^{*} \sinh(2\varepsilon/\varepsilon_{c0}^{*})}}$$
(9)

Here $\sigma'(T)$ is the experimentally measured excess conductivity over the whole temperature interval from T* down to T_c^{mf} . Within the LP model all parameters in (9), including T*, T_c^{mf} , ε , $\xi_c(0)$, A_4 and theoretical parameter ε^*_{01} , can be directly determined from the experiment [2,9,10].

Fig. 3 displays the results of the LP model PG analysis for P=0 GPa, and P=1.05 GPa, curve 1 and 2, respectively. Curve 1 (dots) is computed using Eq.(11) with the following set of parameters derived from experiment: $T^* = 252$ K, $T_{c}^{mf} = 50.2$ K, $\xi_{c}(0) = 3.43$ A, $\epsilon^{*}_{c0} = 0.94$ and $A_{4} = 55$, and curve 2 (semicircles) with T*= 254 K, T_c^{mf} = 56.6 K, $\xi_{c}(0) = 2.91A$, $\varepsilon^{*}_{c0} = 0.71$ and $A_{4} = 100$. Curve 3 is obtained after the polynomial fit of the resistivity data at P=1.05 GPa which we used to avoid the nonphysical jumps of $\Delta^*(T)$ at high temperatures. It is seen in the figure that both curves look rather similar, especially in the range of low temperatures. But both Δ^* BCS and ratio $D^* = 2\Delta^* (T_c^{mf}) / k_B T_c$ noticeably increase with P at a rate dln Δ^* /dP ≈ 0.37 GPa¹, implying an increase of the coupling strength in cuprates with pressure. Found D* = 5 (P=0GPa) and D*=6.6 (P=1.05GPa) correspond to strong coupling limit being typical for HTS's in contrast to BCS weak coupling limit ($2\Delta_0/k_BT_c^{BCS} \approx 4.28$) established for d-wave superconductors [36]. The pressure effect on the PG and D* is observed for the first time.

Obtained dln Δ^* /dP \approx 0.37 GPa⁻¹ is a factor of ~3.3 larger than that reported from tunneling spectra measurements on Ag-Bi2223 point contacts [37] but in a good agreement with results of μ SR experiment on the SD polycrystalline YBa₂Cu₃O_{7-δ}[23]. Simultaneously T_{pair} decreases gradually with P. Eventually, at P=1.05 GPa the Δ^* (T) curve acquires the specific shape with T_{pair} \approx (133+-2) K being typical for the SD YBCO films at P=0 [1,9,10]. This suggests a strong influence of pressure on the lattice dynamics [23] especially in the high-temperature region.

Observed increase of Δ^* and BCS ratio D*, as well as decrease of resistivity, can be accounted for by the anomalous softening of the phonon frequencies under pressure [37]. Correspondingly, observed increase of T_c can be attributed to the rearrangement of the density of charge carriers n_f in conducting CuO₂ planes [22], as mentioned above. It appears that oxygen vacancies in slightly doped cuprates make the n_f rearrangement more easy to achieve.

Conclusion

For the first time the pressure effect on pseudogap $\Delta^{*}(T)$ of slightly doped single crystals of YBa₂Cu₂O_{7.8} was studied within the Local Pair model. Both Δ^* and BCS ratio $D^* = 2\Delta^* (T_c^{mf}) / k_B T_c$ are found to noticeably increase with P at a rate $dln\Delta^*/dP \approx 0.37$ GPa⁻¹, implying an increase of the coupling strength in cuprates with pressure. Simultaneously the sample resistivity ρ is found to decrease with P at a rate $dln\rho(300K)/dP=(-19\pm0.2\%)$ GPa⁻¹ whereas T_c is found to increase at a rate dTc/dP = +5.1 K·GPa⁻¹, which both are in a good agreement with those obtained for the YBCO compounds by different experimental technique. Independently on pressure, near T_c $\sigma'(T)$ is well described by the Aslamasov-Larkin and Hikami-Larkin fluctuation theories demonstrating 3D-2D crossover with increase of T. The crossover temperature T_o determines the coherence length along the c-axis $\xi_{-}(0) = 3.43 \pm 0.02$ Å at P=0 GPa. Revealed value of $\xi_{0}(0)$ is typical for the slightly doped cuprates and is found to decrease with P.

Observed increase of Δ^* and BCS ratio D*, as well as decrease of resistivity, can be accounted for by the anomalous softening of the phonon frequencies under pressure [37]. Correspondingly, observed increase of T_c can be attributed to the rearrangement of the density of charge carriers n_f in conducting CuO₂ planes [22] which is much more easy to obtain in the slightly doped samples.

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